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Science-Based Prediction for Complex Systems

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The topic of this volume, science-based prediction for complex systems, or 'predictive science' for short, is often met with questions. Hasn't science been predictive since the time of Galileo? Haven't we counted on Newton's laws to put a man on the moon and on Maxwell's equations and the constancy of Earth's gravitational field for the fantastic accuracy of the Global Positioning System? So, what's new here, and why has development of predictive capability been named as a primary technical goal of Los Alamos National Laboratory?

Although not entirely new, the pairing of prediction with complex systems makes explicit a growing expectation for accurate predictions, be they about the weather, the growth of foreign markets, or the next moves of terrorist groups. At Los Alamos, the goal is implicit in many aspects of our major missions: from predicting the reliability of our nuclear weapons without further testing to assessing the likely performance over the next 10,000 years of the proposed Yucca Mountain repository for nuclear waste and from developing strategies for detecting the smuggling of nuclear materials to inventing an optimal vaccine strategy for preventing a flu pandemic. The challenges derive not only from the complexity of the problems, but also from the degree of confidence required of the solutions and from the limited data and resources available for solving the problems.

Complex systems, as defined here, involve some combination of nonlinearity, coupled subsystems, and multiple length and time scales. These complexities invariably mean that a system can traverse many different histories, and therefore reliable prediction and accurate assessment of the uncertainties require a probabilistic approach. Also needed are the conscious coordination and integration of experiment, theory, and computer simulation.

At Los Alamos, the major driver for predictive science is, of course, the nuclear weapons program. Since the cessation of testing, the goal of the nuclear weapons program has been to predict the performance of weapons in the stockpile through direct simulation in order to anticipate problems that might arise and then develop efficient ways to fix those problems. In a penetrating analysis that opens this volume, John Pedicini and Dwight Jaeger discuss the new guidance from Washington and then outline the factors that will determine the future nuclear deterrent. What is interesting from the perspective of this volume is the emphasis on increasing predictability by creating a robust replacement for stockpile designs, one with reduced sensitivity to manufacturing and performance variables.

Whatever decisions are made on the future nuclear deterrent, methodologies are needed to predict weapons performance through simulation and to quantify levels of uncertainty. But how does one determine the uncertainties when the simulations contain a maze of errors in input data, physics models, and solution methods? The first article on uncertainty quantification introduces specific methodologies for analyzing simulation errors for multiphysics codes such as those needed for weapons performance. It also applies the methodologies to two real-world problems: estimating the errors in shock propagation problems and predicting production from an oil reservoir. The results provide a compelling case for using error models to estimate uncertainties and, in certain cases, improve the accuracy of the simulations. Using error analysis in a different application, Los Alamos researchers report a remarkable result: a factor of 10 reduction in the uncertainty in the nuclear fission cross section. That reduction is expected to translate into more accurate predictions of weapons performance and better interpretations of past nuclear tests. In the earth sciences, where data are often relatively sparse, uncertainty quantification becomes much less precise. Results reported here on ocean current stability from different ocean models show the real difficulties in predicting global climate change, and examples from volcanology illustrate the types of approximation that feed into practical decision-making.

This volume interprets predictive science in a very inclusive way, by sampling the diverse systems and new approaches being investigated at Los Alamos. The article on networks is a prime example, presenting a new paradigm for describing the interactions in complex systems, whether they consist of people, computers, or the complex molecules of life. The efficiency of information transport on a network seems to strongly influence the network's structural evolution, be it the Internet, the metabolic networks, or a network of scientific collaboration. That idea has led to the solution of several problems, including the design of a computer network for performing agent-based simulations in a scalable fashion.

The article on modeling the response of the retina to visual stimuli outlines another intellectual frontier. Inspired in part by the program to develop a retinal prosthetic for the visually impaired, modeling and experiment have uncovered a mechanism by which the retina may preprocess information on incoming light stimuli. What seems to be a coordinated, context-related neuronal response may also be relevant for understanding the processing that occurs deep within the brain.

Two remarkable developments are reported here on predicting material behavior under extreme conditions. One is predicting the static, dynamic, and optical properties of partially ionized matter using the framework of quantum molecular dynamics. This methodology has correctly predicted the equation of state of hydrogen and of a mixture of nitrogen and oxygen in the shocked state, as well as the viscosity of plutonium. The second development is the validation of material models that predict the deformation and fracture of metals under extreme loading conditions. The extraordinary agreement between simulation and experiment for the degree of strain localization during both tensile tests and explosively driven conditions represents the state of the art in that field.

The problem of predicting turbulence has been recalcitrant to solution for over 80 years. This volume contains an introduction to the problem through the eyes of an experimentalist followed by a discussion of exciting new developments. They include a calculation of the entire turbulent velocity field in a periodic domain, done on the Los Alamos (Advanced Simulation and Computing) Q machine. This calculation shows that the famous Kolmogorov scaling laws hold locally in time but also indicates departures. In fact, a related article on field theory and statistical hydrodynamics reports the first analytical calculation of anomalous scaling in passive scalar turbulence. Also presented is a new model for computing turbulence, known as the LANS-alpha model. Its derivation from Hamilton's principle of least action, the existence and properties of its solutions, its application to benchmark problems, its preservation of properties such as the variability of the flow, and the open problems for increasing its applicability are discussed.

The volume closes with one of the most important efforts related to the accurate simulation of nuclear weapons performance, that of developing numerical methods preserving the most important aspects of the physics. This endeavor began more than 50 years ago, at the inception of electronic digital computers. Here, in a presentation meant to be pedagogical, one gets a glimpse of the creative effort involved in making radiation and hydrodynamic simulations predictive.

All the articles reveal the impact of computational power on the progress toward predictive capability. That power is almost taken for granted, and the center of attention has shifted to what one can do with it, but it is interesting to recall that 30 years ago, when the first Cray computers were delivered to Los Alamos, computing power was less than it is today by a factor of 10^4. Most simulations were one dimensional; that is, they assumed spherical symmetry, and none of the complexity being addressed today was imagined within reach. We've come a long way.

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Los Alamos Science

Science-Based Prediction for Complex Systems

Weapons Outlook

Uncertainty Quantification

Materials

Networks

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Turbulence

Numerical Methods